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*Kurchatov Institute of Atomic Energy, Moscow*[1] *(a)*
*and Institute of Crystallography, Academy of Sciences of the USSR, Moscow*[2] *(b)*

# Bragg-Laue Diffraction in Inclined Geometry

By

P. A. Aleksandrov (a), A. M. Afanasiev (a), and S. A. Stepanov (b)

On the basis of the dynamical theory a new geometry of X-ray diffraction is suggested and analyzed in detail. Diffraction scattering occurs from the planes deviated by several degrees from the surface normal, the incident and diffracted beams forming small glancing angles with the surface. It is shown that the asymmetry factor can be varied within a wide range through small variations of the incidence angle, which makes it possible to study diffraction both in the Laue and Bragg case. A strong dependence is observed of the departure angle of the diffracted wave on the fulfilment of the exact Bragg condition, the angular scale increasing by several orders of magnitude. The possibilities of the above-described geometry for studying thin surface layers are discussed.

Предложена и детально проанализирована на основе динамической теории новая схема дифракции рентгеновских лучей. Дифракционное рассеяние происходит на плоскостях, отклоненных от нормали к поверхности на углы до нескольких градусов, при этом падающий и дифрагированный пучки образуют малые скользящие углы с поверхностью. Показана возможность в широких пределах варьировать фактор асимметрии посредством малых изменений угла падения, изучать дифракцию в геометрии Брэгга, в геометрии Лауэ. Получена сильная зависимость угла выхода дифрагированной волны от выполнения условия Брэгга с увеличением углового масштаба на несколько порядков. Обсуждаются возможности применения новой схемы для изучения тонких поверхностных слоев монокристаллов.

## 1. Introduction

Recent theoretical and experimental studies have shown that X-ray diffraction under specular reflection (SR) conditions is a new, powerful tool for studying the structure of ultrafine layers on a crystal surface. Inclined geometry for the symmetric Laue case has been suggested first in [1] where both the incident and the diffracted beams made small angles with the surface and experienced specular reflection. In [2] the detailed analysis of this geometry was carried out and it was shown that the value of the angle of departure of a specularly reflected diffracted (SRD) wave strongly depends on how accurately the incident beam satisfies the Bragg condition. The ascertainment of this relation provided an essential simplification of the procedure in comparison with that suggested in [1], namely, it was suggested to carry out the experimental measurements using collimation only with respect to the angle of incidence and to separate diffracted rays with different deviations from the Bragg angle not in the plane of diffraction but by measuring their angles of departure from the crystal.

The next step in this direction was made in [3] where the authors used crystals with small misorientation angles, i.e., realized diffraction by planes not exactly normal to the crystal surface. The change in the misorientation angle by several degrees leads

[1]) 123182 Moscow, USSR.
[2]) 59 Leninskii prospekt, 117333 Moscow, USSR.

to qualitatively new results. It turned out that slightly changing the incidence angle, we can observe the transition from the Laue case to the Bragg one, pass from symmetric diffraction to extremely asymmetric diffraction, using the same diffracting planes, and also realize the case where diffraction occurs simultaneously according to Bragg and Laue, which fact is reflected in the title of our paper. In the present work we consistently describe and consider in detail all the cases occurring with inclined geometry, taking into account that the misorientation of several degrees permits us to neglect SR of at least one of the beams.

It is necessary to note that earlier the problem of diffraction by crystals with misoriented surface was considered for a conventional (not inclined) geometry in connection with the great interest in asymmetric monochromators [4 to 14]. In [4 to 6, 10] the Bragg case and in [7, 11, 12] the Laue case was studied. The authors investigated the effect of specular reflection of one of the waves, incident or diffracted, on the shape of the rocking curve and the change in anomalous transmission under the conditions of extremely asymmetric diffraction. It was indicated in [8, 9] that in the extremely asymmetric case both Bragg and Laue diffraction can occur simultaneously.

The interest to the inclined geometry is associated mainly with the possible study of the perfection of very thin subsurface layers of crystals. Since the extinction length is two-to-three orders of magnitude smaller in this case, the diffracted radiation provides direct information on the structure of layers as thick as several nm [15 to 17], while measurements of asymptotic diffraction [18] in the above geometry correspond to the study of monolayers.

## 2. General Equations for Bragg-Laue Diffraction

The geometry of diffraction is shown in Fig. 1. Here $\boldsymbol{\varkappa}_0$, $\boldsymbol{k}_0$, and $\boldsymbol{k}_h$ are the wave vectors of incident, refracted (transmitted), and diffracted waves, respectively, $\boldsymbol{\varkappa}_0^{\mathrm{s}}$ and $\boldsymbol{\varkappa}_h^{\mathrm{s}}$ are the wave vectors of specularly reflected and specularly reflected diffracted waves, $\Phi_0$ is the angle of incidence of the wave onto the crystal, $\Phi_h$ the angle of departure from the crystal of the SRD wave, $\varphi$ the misorientation angle of diffracting planes with respect to the surface normal.

Following [2] and [3], we consider the continuity conditions for the tangential components of wave vectors on the entrance surface of the crystal together with the diffraction conditions. It can readily be obtained that at $\Phi_0$, $\Phi_h$, and $\Psi \ll 1$,

$$\Phi_h^2 = (\Phi_0 + \Psi)^2 - \alpha\,, \tag{2.1}$$

where $\alpha$ is the deviation from the Bragg angle and $\Psi$ is the effective misorientation angle,

$$\alpha = \frac{(\boldsymbol{\varkappa}_0 + \boldsymbol{K}_h)^2 - \varkappa_0^2}{\varkappa_0^2} = -2\sin 2\theta_{\mathrm{B}}(\theta - \theta_{\mathrm{B}})\,, \tag{2.2}$$

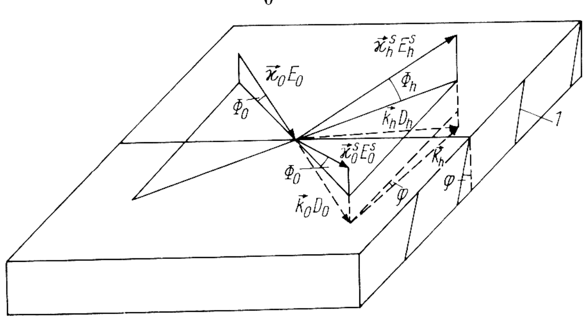


Fig. 1. Bragg-Laue diffraction in inclined geometry. 1 diffracting planes, $\varphi$ misorientation angle, $\Phi_0$ incidence angle, $\Phi_h$ angle of departure of the diffracted beam. For other notations see the text

$\Psi = 2\varphi \sin \theta_B$, angles $\varphi$ and $\Psi$ are considered to be positive, if the reciprocal lattice vector $\boldsymbol{K}_h$ is directed into the crystal.

The equations of the dynamical theory for fields $D_0$ and $D_h$ in the crystal in the case of $\sigma$-polarization have the form

$$\begin{aligned}(u^2 - \Phi_0^2)\, D_0 &= \chi_0 D_0 + \chi_{\bar{h}} D_h\,,\\ [(u + \Psi)^2 - \Phi_h^2]\, D_h &= \chi_0 D_h + \chi_{\bar{h}} D_0\,.\end{aligned} \tag{2.3}$$

Here $u = k_{0z}/\varkappa_0$ is the unknown parameter. In this case the dispersion equation is quartic,

$$(u^2 - \Phi_0^2 - \chi_0)\,[(u + \Psi)^2 - \Phi_h^2 - \chi_0] = \chi_h \chi_{\bar{h}}\,. \tag{2.4}$$

It can be shown that for all values of the parameters the equation has two roots with positive imaginary part and two roots with negative one. Assuming the crystal to be infinitely thick, we must choose roots with positive imaginary parts which correspond to field damping with depth.

To determine the field amplitudes it is necessary to use the boundary conditions on the entrance surface. From the continuity of the tangential components of electric fields it follows

$$\begin{aligned}\Phi_0(E_0 - E_0^s) &= u^{(1)} D_0^{(1)} + u^{(2)} D_0^{(2)}\,,\\ -\Phi_h E_h^s &= (u^{(1)} + \Psi)\, D_h^{(1)} + (u^{(2)} + \Psi)\, D_h^{(2)}\,.\end{aligned} \tag{2.5}$$

The conditions of continuity of the tangential components of magnetic fields are in this case, within the first terms of the expansion in $\Phi_0$ and $\Phi_h$, equivalent to the continuity conditions for the normal components of electric fields,

$$E_0 + E_0^s = D_0^{(1)} + D_0^{(2)}\,, \qquad E_h^s = D_h^{(1)} + D_h^{(2)}\,. \tag{2.6}$$

In these expressions $E_0$ and $E_0^s$ are the amplitudes of incident and specularly reflected waves, $E_h^s$ is the amplitude of the SRD wave.

Solving (2.3) with due account of the boundary conditions (2.5), (2.6) we arrive at

$$E_h^s = \frac{2\Phi_0 W^{(1)} W^{(2)} (u^{(2)} - u^{(1)})\, E_0}{\chi_{\bar{h}}[W^{(2)}(u^{(1)} + \Phi_0)\,(u^{(2)} + \Phi_h + \Psi) - W^{(1)}(u^{(2)} + \Phi_0)\,(u^{(1)} + \Phi_h + \Psi)]}\,. \tag{2.7}$$

Here $W^{(i)} = u^{(i)2} - \Phi_0^2 - \chi_0$ and index $i = 1, 2$ corresponds to two waves being damped with crystal depth, the solutions of dispersion equation (2.4).

Passing to the reflection coefficient, it is necessary to take into account the flux ratio of incident and diffracted beams,

$$P_h^s = \left|\frac{E_h^s}{E_0}\right|^2 \frac{\Phi_h}{\Phi_0}\,. \tag{2.8}$$

The angular dependence of the intensity of SRD wave on $\alpha$ calculated by (2.7), (2.8) can have a shape essentially different from a conventional rocking curve, yet the angular range of the diffraction maximum is approximately the same, several seconds of arc. If the same intensity is considered as a function of the angle of departure from the crystal, $\Phi_h$, and (2.1) relating $\alpha$ with $\Phi_h$ is taken into account, the angular scale increases by several orders of magnitude,

$$\delta\Phi_h = -\frac{\delta\alpha}{2\Phi_h} \approx \frac{-\delta\alpha}{2|\Phi_0 + \Psi|} \approx (10^1 - 10^3)\,\delta\alpha\,. \tag{2.9}$$

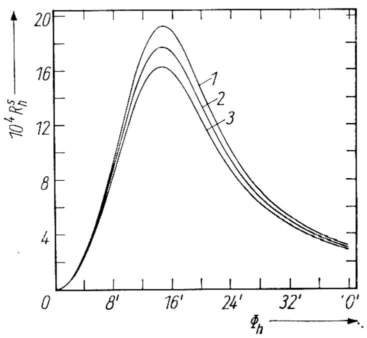


Fig. 2. The effect of small misorientations on the intensity of diffracted curves. Si(220) $\mathrm{CuK}_\alpha$, $\Phi_0 = 13.34'$, misorientations (1) $\varphi = -1'$, (2) $\varphi = 0'$, (3) $\varphi = +1'$

Clearly, that such a gain in the angular scale is possible only at small angles $\Phi_0$, $\Phi_h$, and $\Psi$.

It is also obvious that independently of the fact whether intensities are measured depending on $\alpha$ or $\Phi_h$ the integral intensity should be the same, and, consequently, the reflection coefficient $R_h^s$ will be renormalized when measurements are taken depending on $\Phi_h$,

$$R_h^s = 2\Phi_h P_h^s \,, \tag{2.10}$$

where the factor $2\Phi_h \approx 10^{-1}$ to $10^{-3}$ corresponds to the lower density of states for the dependence of the intensity on the angle of departure.

In the absence of misorientation ($\Psi = 0$) (2.7) transforms into the formula for diffraction from crystals without misorientation [2]. An important factor, characteristic of the geometry used and following from the obtained relationships, is a high sensitivity to small misorientations comparable with the critical angle of the total external reflection, $\Phi_c = \sqrt{|\chi_0|}$. Fig. 2 shows curves $R_h^s(\Phi_h)$ calculated for Si(220) $\mathrm{CuK}_\alpha$ reflection, $\Phi_0 = \Phi_c = 13.34'$ for three different values of misorientation, $\varphi = 0', \pm 1'$. It is seen that misorientation as small as $1'$ corresponds to a 10% change in intensity. These data prove, firstly, that it is possible to measure with precision the misorientation angle from the difference of the intensities of $hkl$ and $\bar{h}\bar{k}\bar{l}$ reflections from the misoriented plane and, secondly, that one should have very flat surfaces for experimental work in inclined geometry.

Crystals with quite a considerable misorientation can give a large amount of various diffraction curves which will be classified and considered in detail later on.

## 3. Diffraction Geometry Depending on Incidence Angle

The geometry described in [1, 2] corresponds to symmetric diffraction in the Laue case ($\Psi = 0$). The reciprocal lattice vector is parallel to the crystal surface. The diffracted wave $\boldsymbol{k}_h$ receives no additional momentum directed into the crystal or towards the entrance surface.

If the reciprocal lattice vector is misoriented in such a way that its normal component is directed into the crystal ($\Psi > 0$), we have asymmetric diffraction in the Laue case. Then the diffracted wave $\boldsymbol{k}_h$ receives an additional momentum directed into the crystal and the angle between the wave and the surface increases, whereas the intensity of the SRD wave decreases.

The most interesting cases are those characterized by large negative misorientations ($\Psi < 0$, $\Phi_c \ll |\Psi| \ll 1$). During such reflection the diffracted wave $\boldsymbol{k}_h$ receives an additional momentum in the direction of the external normal to the surface, therefore the diffraction geometry depends on the incidence angle. At small incidence angles ($\Phi_0 < |\Psi|$) Bragg-case diffraction occurs, while at large ones ($\Phi_0 > |\Psi|$) diffraction according to Laue is observed. At $|\Psi| - \Phi_c \leqq \Phi_0 \leqq |\Psi| + \Phi_c$ the Bragg case changes to the Laue case. In the Bragg case the wave $\boldsymbol{k}_h$ in the crystal is directed towards the entrance surface, and the wave $\boldsymbol{\varkappa}_h^s$ is its refracted continuation in vacuum and not the specular component as it takes place in the Laue case.

A remarkable property of the inclined geometry in the Bragg case is the possibility to vary within a wide range the asymmetry factor by slightly changing the incidence angle. At $0 < \Phi_0 \leqq \Phi_c$ we obtain extremely asymmetric inclined Bragg-case diffraction with specular reflection of the incident beam $\beta = \Phi_0/(|\Psi| - \Phi_0) \ll 1$. With an increase in the incidence angle the asymmetry becomes less pronounced and the value $\Phi_0 = 0.5\,|\Psi|$ corresponds to the symmetric, inclined diffraction in the Bragg case, $\beta = 1$. In this case neither of the beams experiences SR, since $\Phi_0$, $\Phi_h \gg \Phi_c$. Increasing further $\Phi_0$ at $0 < |\Psi| - \Phi_0 \leqq \Phi_c$ we observe again an extremely asymmetric Bragg pattern, $\beta \gg 1$ near the Bragg-Laue transition, the conditions of SR for the diffracted wave being fulfilled.

On the whole, the asymmetry factor in the region under consideration varies within the limits

$$\frac{\Phi_c}{|\Psi| - \Phi_c} < \beta < \frac{|\Psi| - \Phi_c}{\Phi_c}. \tag{3.1}$$

Thus, in Si(111) wafers with maximum 4° misorientation along the $[11\bar{2}]$ direction there are $(01\bar{1})$ planes with 3°38′ misorientation. Using the second order of the $\mathrm{CuK}_\alpha$ reflection from these planes, we obtain $\Psi = -166.6'$, $\Phi_c = 13.3'$, and $0.08 < \beta < 12.00$, i.e., $\beta$ may vary within a wide range.

Still further increasing the incidence angle, $\Phi_0 > |\Psi|$ leads to the transition to an extremely asymmetric Laue case, i.e. the diffracted beam propagates into the crystal. If the incidence angle is within the interval $\Phi_0 \sim |\Psi| \pm \Phi_c$, the condition for SR is fulfilled and we observe an SRD wave. The wave diffracted according to Bragg, $\varkappa_h^s$, transforms into the specular component of the wave diffracted according to Laue. As has been shown in [2] the intensity of the SRD wave in this case, similar to the Bragg case, is comparable with the intensity of the incident wave. For larger incidence angles the SRD wave starts damping as $1/\Phi_0^4$, the asymmetry becomes less pronounced and Laue case diffraction occurs with slight asymmetry.

The absence of SR for at least one of the waves provides an essential simplification of the general relationships obtained in Section 2 for each of the cases.

## 4. Transformation of Dispersion Equation

For further consideration it is convenient to introduce new variables into the dispersion equation (2.4).

Let us introduce instead of $u$ the following parameters:

$$\begin{aligned} S_0 &= u - \sqrt{\Phi_0^2 + \chi_0}\,, \qquad S_0^s = u + \sqrt{\Phi_0^2 + \chi_0}\,, \\ S_h &= u + \Psi - \sqrt{\Phi_h^2 + \chi_0}\,, \qquad S_h^s = u + \Psi + \sqrt{\Phi_h^2 + \chi_0}\,. \end{aligned} \tag{4.1}$$

These variables characterize the change in the normal component of the wave vector in a crystal at diffraction. The position of a diffraction maximum in the Bragg case corresponds to $S_0 = S_h^s$ and in the Laue case to $S_0 = S_h$. A small value of the quantity $|S_0^s| \leqq \Phi_c$ corresponds to the intensive excitation of the specularly reflected wave $E_0^s$.

Conditions $S_0 = S_h$ and $S_0 = S_h^s$ determine the angular shift of the diffraction maximum due to refraction from the position $\alpha = 0$ predicted by the kinematical theory. Let us introduce a complex parameter $\tilde{\alpha}$ to describe the shift. According to (4.1) and (2.5), we obtain

$$\tilde{\alpha} = \alpha - 2\Psi(\Phi_0 - \sqrt{\Phi_0^2 + \chi_0}) \tag{4.2}$$

(Re $\tilde{\alpha} = 0$ determines the angular position of the maximum). It should be noted that the position of the intensity maximum of the wave $\varkappa_h^s$ coincides with the position of the diffraction maximum only in the Bragg case. For the Laue case the position of the intensity maximum from the side of the entrance surface is determined mainly by the angular dispersion of SR and not by diffraction scattering.

At large angles $\Phi_0$, $\Phi_h \gg \Phi_c$ (4.2) reduces to the standard one (see, e.g., [19]),

$$\tilde{\alpha} = \alpha - \chi_0\left(1 \mp \frac{\Phi_h}{\Phi_0}\right), \tag{4.3}$$

where plus corresponds to the Bragg case, $\Phi_0 + \Psi < 0$.

The dispersion equation in the new notation has a rather simple form

$$S_0 S_h S_0^s S_h^s = \chi_h \chi_{\bar{h}} \tag{4.4}$$

or

$$S_0(S_0 + \sqrt{\Phi_0^2 + \chi_0} + \Psi - \sqrt{\Phi_h^2 + \chi_0})\,(S_0 + 2\sqrt{\Phi_0^2 + \chi_0})\,(S_0 + \sqrt{\Phi_0^2 + \chi_0} + {}$$
$$+ \Psi + \sqrt{\Phi_h^2 + \chi_0}) = \chi_h \chi_{\bar{h}}\,. \tag{4.4a}$$

Now, it is easy to see the approximate solutions of the dispersion equation. In the zeroth approximation ($\chi_h = 0$) four roots $S_0^{(i)}$ of (4.4) correspond to successively vanishing multipliers in the left-hand side. If for one of the roots the remaining multipliers turn out to be much larger than $\sqrt{|\chi_h|}$ the root can readily be calculated and the degree of the equation reduces by one. If we obtain two such roots, the dispersion equation reduces to a quadratic one. Below we shall show that in the case of SR for the incident and diffracted waves the equation is quartic; if SR occurs only for the incident or diffracted wave the equation is cubic; if there is no SR the equation is of second order.

## 5. Inclined Bragg Diffraction without Specular Reflection

Let us consider in more detail diffraction at incidence angles satisfying condition (3.1) where we can neglect SR for both the incident and diffracted waves. The dispersion equation has two solutions with waves damping with the crystal depth, $S_0^{(1)} = 2\Phi_h$ and $S_0^{(2)}$, the latter satisfying the equation

$$S_0\left(S_0 + \frac{\tilde{\alpha}}{2\Phi_h}\right) + \frac{\chi_h \chi_{\bar{h}}}{4\Phi_0 \Phi_h} = 0 \tag{5.1}$$

and condition (see (4.1))

$$\mathrm{Im}\,(S_0^{(2)} + \sqrt{\Phi_0^2 + \chi_0}) > 0\,. \tag{5.2}$$

The corresponding solution is

$$S_0^{(2)} = \frac{\sqrt{\chi_h \chi_{\bar{h}}}}{2\Phi_h \sqrt{\beta}}\,\left(-y \pm \sqrt{y^2 - 1}\right), \tag{5.3}$$

$$y = \frac{\tilde{\alpha}\sqrt{\beta}}{2\sqrt{\chi_h \chi_{\bar{h}}}}. \tag{5.4}$$

Parameters $W^{(i)}$ entering (2.7) have the form

$$W^{(i)} = S_0^{(i)}\left(S_0^{(i)} + 2\sqrt{\Phi_0^2 + \chi_0}\right). \tag{5.5}$$

Since $|W^{(1)}| \gg |W^{(2)}|$, the expression for the amplitude $E_h^s$ is essentially simplified and we arrive at

$$E_h^s = \frac{W^{(2)}}{\chi_{\bar{h}}} E_0 \approx \frac{2\Phi_0}{\chi_{\bar{h}}} S_0^{(2)} E_0 . \tag{5.6}$$

Substituting the latter expression into (2.8), we obtain the well-known expression of the dynamical theory

$$P_h^s = \left|\frac{\chi_h}{\chi_{\bar{h}}}\right| |-y \pm \sqrt{y^2 - 1}|^2 . \tag{5.7}$$

Let us consider this expression from a somewhat different standpoint. It has already been indicated how important it is to use small angles $\Phi_0$ and $\Phi_h$ in the given geometry. Due to the relation between $\Phi_0$, $\Phi_h$, and $\alpha$, we study the rocking curves taken depending on the angle of departure $\Phi_h$ and not on $\alpha$, as in the conventional methods. The halfwidth of the Darvin curve, $\Delta\Phi_h$, determined from the condition $y = \pm 1$ is

$$\Delta\Phi_h = \frac{2|\chi_h|}{\sqrt{\Phi_0 \Phi_h}} . \tag{5.8}$$

For example, for Si(111) for the symmetric (220) $\mathrm{CuK}_\alpha$ reflection ($\Phi_0 = 83.3'$) $\Delta\Phi_h = 160''$, whereas using the conventional recording depending on $\alpha$, we have $\Delta\theta = 6.7''$. The shape of the diffraction maximum for recording with respect to $\Phi_h$ is shown in Fig. 3 (the calculations were performed by the general formulae (2.7, 2.8)).

Thus, the use of small angles provides an essentially higher accuracy of measuring rocking curves. Such an attempt was made first in [20]. It is clear that the diffraction pattern is described by the approximate formula (5.7) until $\Phi_h \gg \Phi_c$, i.e. for $\alpha \ll \ll (|\Psi| - \Phi_0)^2$.

Another specific feature of using small angles is an essential decrease in the extinction length. It can readily be estimated that the amplitude of the field corresponding to the root $S_0^{(1)}$ is small,

$$\left|\frac{D_h^{(1)}}{D_h^{(2)}}\right| = \left|\frac{S_0^{(2)}}{2\Phi_h}\right| \sim \left|\frac{\Phi_c}{\Psi}\right|^2 \ll 1 . \tag{5.9}$$

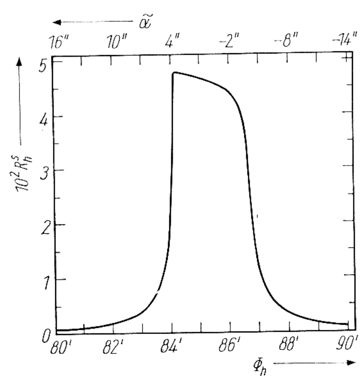


Fig. 3. Diffraction curve taken depending on the angle of departure for the symmetric Bragg case. Si(220) $\mathrm{CuK}_\alpha$, $\Psi = -166.61'$, $\Phi_0 = 0.5\,|\Psi|$. The corresponding angular scale with respect to $\tilde{\alpha}$ is shown in the upper part of the drawing

Therefore, neglecting the field $D_h^{(1)}$, we obtain for the extinction length corresponding to the field $D_h^{(2)}$,

$$L_{ex} = \left. \frac{\lambda}{2\pi \operatorname{Im}\left(S_0^{(2)} + \dfrac{\chi_0}{2\Phi_0}\right)} \right|_{y=0} \approx \frac{\lambda}{\pi} \frac{\sqrt{\Phi_0 \Phi_h}}{|\chi_h|}; \tag{5.10}$$

According to this relationship, the extinction length in the inclined Bragg geometry can be $\approx 50$ times less as compared with the conventional case. Thus, for silicon (5.10) gives in our case $L_{ex} = 130$ nm. This value exceeds that for diffraction under SR conditions ($\approx 10$ nm). However, in the case of SR an additional wave field with large penetration depth appears in the crystal, which complicates the picture [15]. Thus, the inclined Bragg diffraction providing small penetration depth and simple interpretation of the results obtained, permits one to study very thin surface layers of crystals.

### 6. Inclined Bragg Diffraction under Specular Reflection Conditions

At small incidence angles $\Phi_0 \sim \Phi_c$ specular reflection takes place only for the incident wave. Taking into account that $\Phi_h \gg \Phi_c$, we can eliminate one root, $S_0^{(1)} = |\Psi| + \Phi_h$ and to reduce the degree of equation (4.4) by one,

$$S_0\left(S_0 + \sqrt{\Phi_0^2 + \chi_0} + \Phi_h - |\Psi|\right)\left(S_0 + 2\sqrt{\Phi_0^2 + \chi_0}\right) = \frac{-\chi_h \chi_{\bar{h}}}{\Phi_h + |\Psi|}. \tag{6.1}$$

Here only one root $S_0^{(2)}$ corresponds to the damping of fields with crystal depth. Since $|S_0^{(2)}| \ll |S_0^{(1)}|$, (2.7) acquires a simple form,

$$E_h^s = -\frac{\chi_h \Phi_0}{\Phi_h\left(S_0^{(2)} + \sqrt{\Phi_0^2 + \chi_0} + \Phi_0\right)\left(S_0^{(2)} + \sqrt{\Phi_0^2 + \chi_0} + \Phi_h - |\Psi|\right)} E_0 . \tag{6.2}$$

In this case an essential contribution to the diffracted wave comes from only one wave field. This statement concerns the wave $E_0^s$ too.

Of greater interest is the case of large incidence angles near the Bragg-Laue transition where $\Phi_h \sim \Phi_c$, i.e., the condition of SR is fulfilled for the diffracted wave. The dispersion equation in this case is cubic,

$$S_0[S_0^2 - 2S_0(|\Psi| - \Phi_0) + \tilde{\alpha}] = \frac{\chi_h \chi_{\bar{h}}}{2\Phi_0}. \tag{6.3}$$

Equation (6.3) has two roots $S_0^{(1,2)}$ satisfying condition (5.2) and the third root $S_0^{(3)}$ corresponding to the wave not being damped with the crystal depth. From (2.7) one can readily obtain

$$E_h^s = \frac{\chi_h E_0}{S_0^{(3)}(S_0^{(3)} + \Phi_0 - |\Psi| - \Phi_h)}. \tag{6.4}$$

It is worth noting that the field amplitude is expressed through root $S_0^{(3)}$. Both fields $S_0^{(1,2)}$ give comparable contributions to $E_h^s$.

Relations (6.3), (6.4) describe in a rather simple way the transition from the Bragg to the Laue case in inclined geometry. Fig. 4 shows the results of the calculations for Si(220) $CuK_\alpha$ with the misorientation parameter $\Psi = -166.6'$. With an increase in the incidence angle from 150′ to 170′ the diffraction maximum shifts towards lower angles of departure and its amplitude substantially decreases. It is important that no anomalies in the Bragg-Laue transition were observed and the transition occurs continuously. Indeed, at angles $\Phi_h \lessapprox \Phi_c$ the second wave field is intensively excited

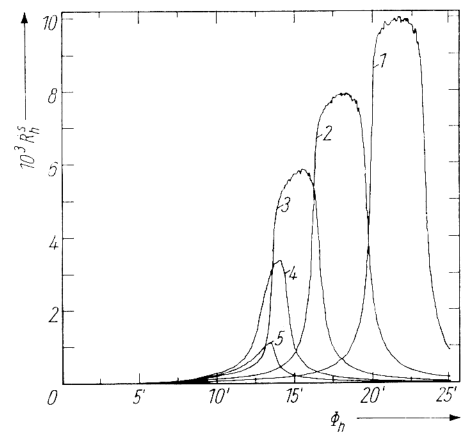


Fig. 4. The Bragg-Laue transition depending on the variation in the incidence angle. Si(220) $CuK_\alpha$, $\Psi = -166.61'$, (1) $\Phi_0 = 150'$, (2) $\Phi_0 = 155'$, (3) $\Phi_0 = 160'$, (4) $\Phi_0 = 165'$, (5) $\Phi_0 = 170'$

in the crystal. The transition for these fields occurs at different values of $\Phi_0$ and $\Phi_h$ Moreover, the relation between $\Phi_0$, $\Phi_h$, and $\alpha$ leads to the dependence of the transition angle on $\alpha$ and to a larger spread of the transition. At $\Phi_0 \sim |\Psi| \pm \Phi_c$ the wave $\varkappa_h^s$ is transformed into a specular component of the diffracted wave whereas the wave $\boldsymbol{k}_h$ itself penetrates into the crystal depth.

As has already been noted, the main advantage of the inclined geometry in the study of the Bragg-Laue transition consists in the possibility of varying the asymmetry factor through small changes in the incidence angle. The experimental studies of this transition in standard (not inclined) geometry [13, 14] meet great difficulties. In [13] the experiment on white neutron-beam scattering was described. The authors have analyzed the Bragg-Laue transition since it was possible to record both Bragg and Laue cases for the scattered radiation. In [14] the crystal was rotated around the reciprocal lattice vector to vary the asymmetry factor in an extremely asymmetric geometry, which resulted in the Bragg-Laue transition due to the deviation of the scattering plane from the surface normal. Our approach is close to that used in [14] whose authors unfortunately used the formulae derived for the case with no inclination [10] without theoretical foundation. Moreover the use of large incidence angles hinders the characterization of thin surface layers.

## 7. Diffraction Curves Taken Depending on $\alpha$

It has already been noted that in diffraction by crystals without misorientation the measurements of diffraction curves depending on $\alpha$ are associated with great experimental difficulties since collimation is necessary both with respect to $\alpha$ and $\Phi_0$. Thus, in [1] collimation with respect to $\alpha$ was realized with the aid of a bent graphite monochromator, while collimation with respect to $\Phi_0$ with the use of slits with an accuracy of $\approx \Phi_c$, which naturally decreased the total experimental accuracy. If there is misorientation equal to several degrees, the incidence angle can be chosen sufficiently large and the requirements to collimation with respect to $\Phi_0$ are not so severe. Therefore, measurements with respect to $\alpha$ can be taken with sufficient accuracy.

Now, consider in more detail the specific character of diffraction curves with respect to $\alpha$ in the inclined geometry. At $\alpha < 0$ the rocking curves fall off as $|\alpha|^{-3/2}$, whereas at $\alpha > 0$ they terminate at the critical angle

$$\alpha_c = (\Phi_0 + \Psi)^2 \tag{7.1}$$

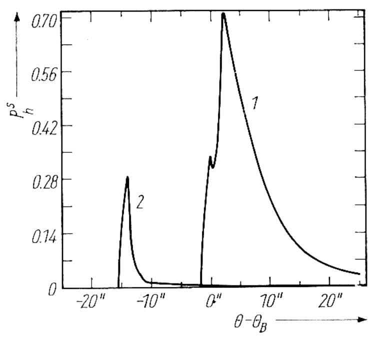


Fig. 5. Intensity versus $\alpha$ for positive and negative misorientations. Si(220) $CuK_\alpha$, $\Phi_0 = 12'$, (1) $\Psi = +24'$ (Laue case), (2) $\Psi = -24'$ (Bragg case)

at which the diffracted wave experiences total internal reflection from the surface and cannot leave the crystal. This phenomenon has been noticed in studies of non-inclined, extremely asymmetric diffraction [8, 9].

At $\alpha > \alpha_c$ the angle $\Phi_h$ is imaginary, and a more general expression should be used instead of (2.8),

$$P_h^s = \left|\frac{E_h^s}{E_0}\right|^2 \frac{\mathrm{Re}\,\Phi_h}{\Phi_0}. \tag{7.2}$$

Curves taken with respect to $\alpha$ are shown in Fig. 5. Note, that in the Laue case the intensity maximum is noticeably shifted and is fully determined by SR. One can observe no peaks at $\tilde{\alpha} = 0$ on this curve. In the Bragg case SR results in the appearance of an additional maximum at small angles of departure.

The region near $\alpha_c$ is characterized by total external reflection at small $\Phi_0$, on the one hand, and, on the other hand, by total internal reflection. In [21, 22] this fact was interpreted as the presence of an X-ray surface wave. But in the actual fact such an interpretation has no grounds. Surface waves are usually called the waves which freely or with insignificant damping propagate along the surface, i.e., the waves which are the eigen-solutions of the problem. The most appropriate example here is that of polaritons. In our case to obtain a wave propagating along the surface (the diffracted wave), it is necessary also to have simultaneously the transmitted wave. These two waves are dynamically related and they are "fed" by the wave incident onto the crystal. Hence, it follows that the surface wave cannot exist by itself, i.e., it is not an eigen-solution. This should be kept in mind if one wants to use this phenomenon for surface characterization [22] and designing gamma lasers [23].

As has already been indicated, of great interest for studying surface layers is the measurement of asymptotic diffraction in inclined geometry. The diffraction is called asymptotic if there are significant deviations from the diffraction maximum [18]. As has been shown in [18], though the penetration depth of X-ray radiation in a crystal at large values of $\alpha$ reaches the value of the absorption depth, the diffracted radiation escapes effectively from a layer of thickness $z \sim \lambda/|\alpha|$. It can readily be shown that at $|\alpha| \gg \Psi^2$ in the inclined geometry the excape depth in asymptotic diffraction is $z \sim \lambda/\sqrt{|\alpha|}$. Thus in the case of inclined geometry a certain depth can be reached at smaller values of $\alpha$, the intensity losses being smaller. Thus at $\alpha \approx 40'$ in the ordinary Bragg case $z \approx 100\lambda$, whereas in inclined geometry $z \approx 10\lambda$, which provides the study of monolayers.

## 8. Conclusion

The above analysis of diffraction scattering in Bragg-Laue geometry provides great possibilities of using such diffraction. First and foremost, it concerns the study of structural perfection of thin surface layers of crystals. The high sensitivity of the method to the presence of an amorphous film on the crystal surface has been demonstrated in [17, 20, 24, 25]. Another aspect of the above-considered diffraction geometry is the possibility of measuring small misorientations of the crystal surface with respect to the crystallographic planes. It is also possible to measure surface bending and roughness. Of significant interest is also the measurement of diffraction curves depending on the angle of departure. An increase of the angular scale by several orders of magnitude would essentially simplify to take diffraction curves proper and would provide highly accurate measurements of structure amplitudes.

In conclusion, we should like to consider the applicability of the kinematical approach to the diffraction in the inclined Bragg-Laue geometry. Vineyard [26] has developed the theory of diffraction under the conditions of specular reflection on the basis of the distorted wave approximation. In this approximation refraction and reflection of waves from the crystal surface is described by the Fresnel formulae, while diffraction scattering of refracted waves in the crystal is taken into account kinematically, since it is assumed that for small penetration depths of a radiation in a crystal, which is associated with total external reflection, the processes of multiple diffraction scattering are not essential. The dynamical consideration [2, 15] disprove this assumption — excitation in a crystal under the conditions of total external reflection of the second wave field with a considerable penetration depth and close values of the amplitudes of reflected diffracted and incident waves — evidence the presence of dynamical diffraction scattering.

Therefore, a more general dynamical approach should be invoked, whereas the kinematical approximation can be used for curve tails or in the cases of strong disturbances.

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